

Auramine
492-80-8 | DTXSID7043821

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.79e-03 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.08e-01

Confidence level: 4.17e-01

Nearest Neighbors from the Training Set

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1,3-Diphenylguanidine

Measured: 4.73e-03

Predicted: 2.00e-03

Image not found

Dodine

Measured: 2.77e-03

Predicted: 2.87e-03

Image not found

Dodine

Measured: 2.19e-03

Predicted: 2.87e-03

Image not found

Guanidine, N,N^{'''}-(iminodi-8,1-octanediyl)bis-

Measured: 2.15

Predicted: 9.84e-01